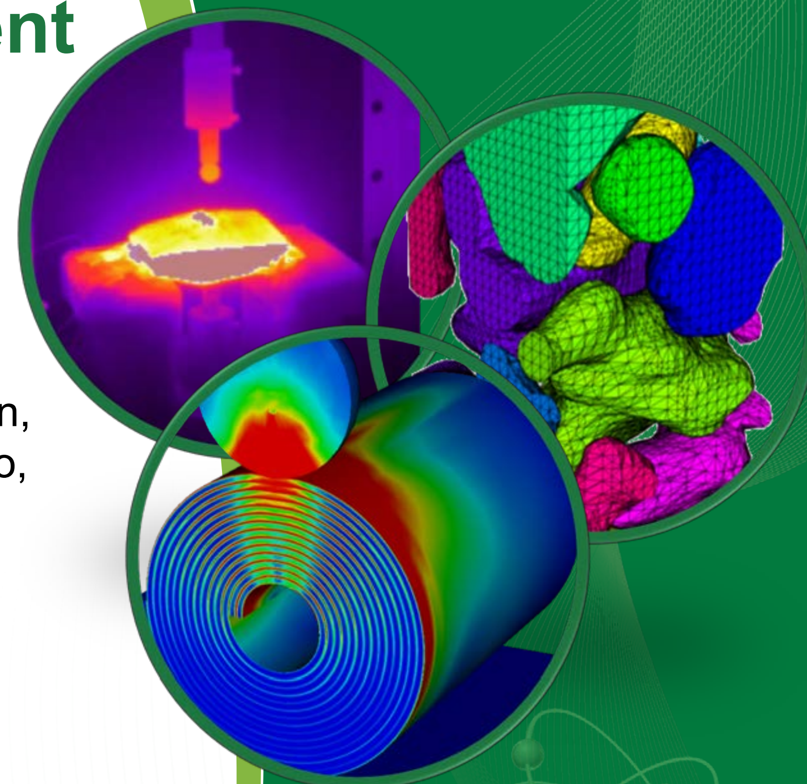
Enhancement and Deployment of VIBE, the Open Architecture Software (OAS) Environment



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2017 U.S. DOE Vehicle Technologies Office Annual Merit Review

June 6, 2017 **Project ID:** ES300

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

- Start
  - October 2015
- Finish
  - September 2018
- Percent complete: 55%

Barriers Addressed

C. Performance
D. Abuse Tolerance, Reliability, and Ruggedness
E. Life

Budget

- FY16
  - Total CABS Funding: 2,265K
  - This effort: 613K
- FY17
  - Total CABS Funding: 2,225K
  - This effort: 570K

Partners

- LBNL
- SNL
- ANL
- as well as the NREL-led CAEBAT project team

Relevance and Project Objectives

- Major barriers for increasing battery energy density and power, increasing safety and reducing cost include
  1. insufficient understanding of the underlying physical phenomena that limit battery performance and safety
  2. lack of validated predictive simulation tools.

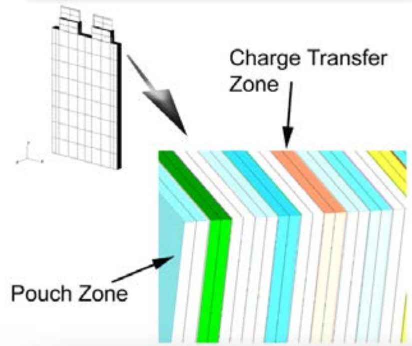
- CABS is addressing (1) by developing new experiments for properties with largest uncertainties and developing new validated models that allow researchers to explore battery response under both normal and abusive conditions, and is addressing (2) by deploying increasingly capable and computationally efficient releases of the Open Architecture Software (OAS) and components of the Virtual Integrated Battery Environment (VIBE), developed as part of CAEBAT.

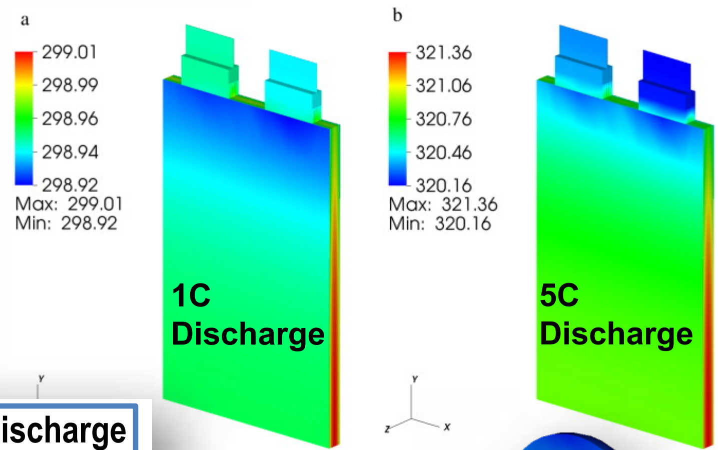
Milestones (FY16)

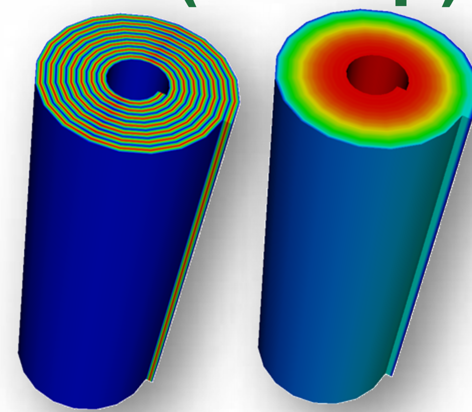
IDs indicate whether milestones are primarily experimental (E), computational (C), or integrated (I).							
ID	FY16	Lead	Q1	Q2	Q3	Q4	Status
C.1	Baseline performance profile of VIBE/OAS/AMPERES	ORNL	P				Complete
I.1	Report on experimental techniques supporting models	ORNL		P			Complete
E.1	Produce segmented tomographic reconstructions of electrodes for conversion to spatial domains for microstructural models	LBNL			P		Complete
E.2	Demonstration of single side indentation test with incremental deformation to determine faulting in spirally wound, wound prismatic, and stacked electrodes in hard case	ORNL				P	Complete
C1.1	Collect constitutive models for NMC materials and report on use of mesoscale data to project lead.	SNL				P	Complete
I.2	Deployment of VIBE/OAS with enhanced extensibility and hybrid models	ORNL				S	Complete

Virtual Integrated Battery Environment (Recap)

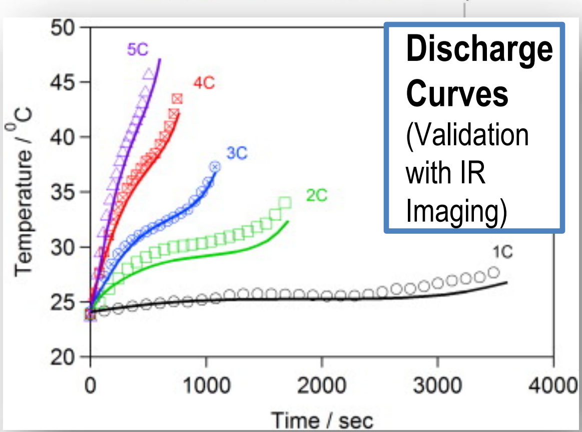
Detailed 3D Modeling

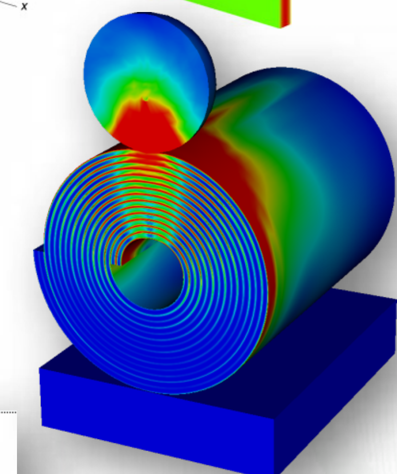




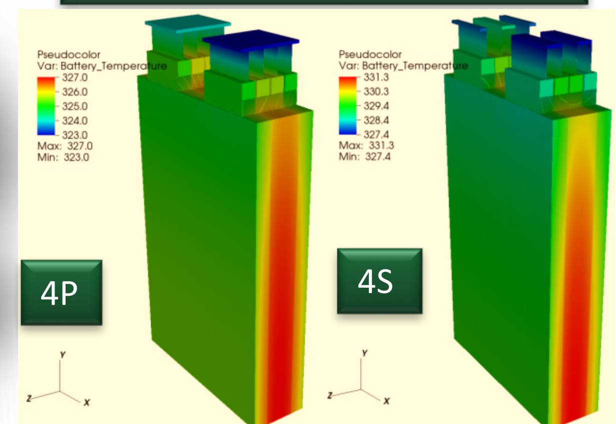


Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal - Electrical)





Mechanical Abuse of Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal – Electrical – Mechanical)



Temperature in 4P and 4S Module with Fully Coupled Electrochemical, Electrical and Thermal Simulations in CAEBAT OAS / VIBE

ELSEVIER
Journal of Power Sources
Available online 24 August 2013
In Press, Accepted Manuscript — Note to users

A new open computational framework for highly-resolved coupled 3D multiphysics simulations of Li-Ion Cells ☆

Srikanth Allu, Sergiy Kalnaus, Wael Elwasif, Srdjan Simunovic, John Turner, Sreekanth Pannala
Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831

Approach: "Traditional" VIBE Components

- Python wrappers that plug into OAS framework
- Expose uniform, lite interface
  - `init() - step() - finalize()`
- Invoked by a simulation driver in a time loop
- Stepping through simulation time steps involves complete execution of underlying code
  - Can be expensive if code operations DO NOT depend on changes to the battery state (e.g. meshing)
- Solution
  - Restructure component/code to avoid repeating operations unnecessarily

Approach : Continuous Execution VIBE Physics Based Software Components

- Launch underlying code as a Daemon i.e., as an independent background process
- Python component wrapper translates calls from simulation driver into messages to the daemon
- Underlying code can maintain state in-memory across time steps and startup cost paid only once
- Client/Server setup
  - C++ library to streamline code communication with Python component with a simple interface: **`getCommand() / sendResponse()`**
- New Python component wrappers
  - Drop in replacement for "traditional" VIBE components
  - One line change in the configuration file thanks to OAS/VIBE component-based design.

Technical Accomplishments: Continuous Execution profiling

Time Step	NTG	TH	EL:	TH:PO	TH:PI	NTG:PO	NTG:PI	EL:PO	EL:PI	Total
1	1.78	90.73	81.28	2.6	2.44	3.82	2.33	2.46	2.28	**189.72**
2	1.77	26.7	39.53	2.56	2.47	3.8	2.33	2.41	2.3	**83.87**
3	2.12	26.56	39.98	2.58	2.29	3.66	3.11	2.89	2.61	**85.8**
4	1.78	26.71	39.21	2.54	2.32	3.69	2.41	2.52	2.28	**83.46**
5	1.77	26.86	39.17	2.5	2.36	3.69	2.39	2.41	2.51	**83.66**
6	1.74	26.73	39.59	2.51	2.24	3.69	2.29	2.36	2.27	**83.42**
7	1.77	26.82	39.16	2.51	2.24	3.74	2.34	2.38	2.26	**83.22**
8	1.73	26.67	39.15	2.5	2.28	3.77	2.32	2.41	2.26	**83.09**
9	1.81	27.19	39.39	2.48	2.25	3.7	2.35	2.39	2.37	**83.93**
Total	**16.27**	**304.97**	**396.46**	**22.78**	**20.89**	**33.56**	**21.87**	**22.23**	**21.14**	**860.17**
%	**1.81%**	**33.98%**	**44.18%**	**2.54%**	**2.33%**	**3.74%**	**2.44%**	**2.48%**	**2.36%**	**95.84%**

Driver Setup	Solve	Compute T Average	Total
60.705	12.037	14.28	87.022
	12.015	13.87	25.885
	12.105	13.6	25.705
	12.076	13.91	25.986
	12.162	14	26.162
	12.079	13.93	26.009
	12.102	13.98	26.082
	12.106	13.87	25.976
	12.117	14.21	26.327

Driver Setup	Solve	Compute Sources	
39.234	8.574	30.373	78.181
	8.562	30.898	39.46
	8.563	31.09	39.653
	8.549	30.602	39.151
	8.562	30.552	39.114
	8.548	30.979	39.527
	8.562	30.528	39.09
	8.561	30.521	39.082
	8.562	30.695	39.257

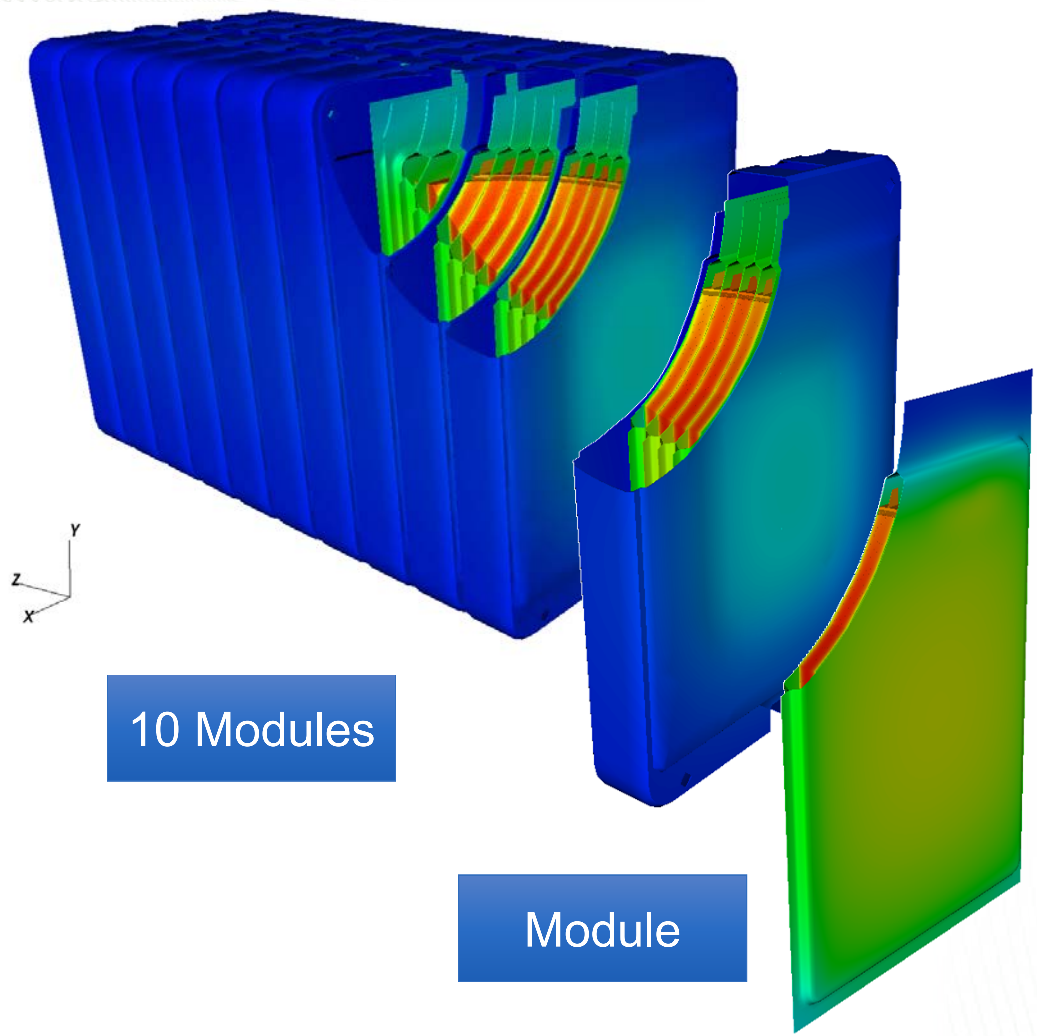
49 % ↓ sim time

Technical Accomplishments: Deployment of software

- Latest software release through standard Virtual Machine (VM)
  - VIBE software is available to download from http://batterysim.org
  - Updated the release document describing new features
  - Completely tested various support cases as part of the release

- Testing new software packing tools : Docker container
  - Makes the UserInterface(ICE) native client
  - Allows user to port the data/meshes in single step
  - Deployment of the container should be straight forward b/w desktop to hpc platform

Technical Accomplishments:

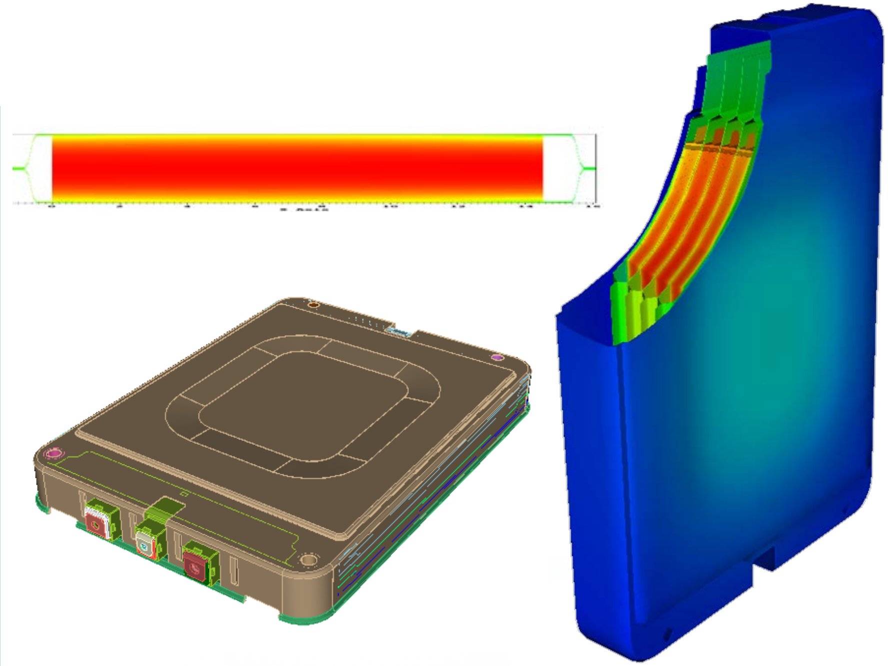


- Fully resolved electrode thickness over all the cells in a battery pack with a total of 16 million degrees of freedom
- Coupled Electro-chemistry and Thermal transport for NMC/Graphite electrodes
- Test cases of coupled electrochemical-thermal simulation for hybrid pulse power characterization of the battery module
- Capability to setup variable potentio-static, galvano-static and open circuit voltage(OCV) resting conditions

Summary Milestone-I.2 (Status: Complete)

Goals

- Software design updates to improve VIBE computational performance
  - Continuous execution of physics based solver components
- Capability to simulate dynamic discharge
  - Coupled electrochemical-thermal simulations under variable potentio-static / galvano-static conditions
- Deployment of the software



Approach / Strategy

- Launch component as daemon
- Python component wrapper translates calls from simulation driver into messages to daemon
- Deployment via docker container

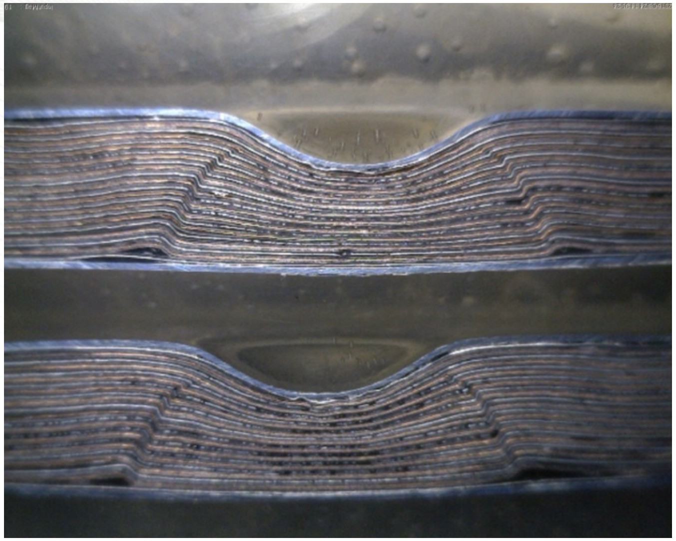
Results

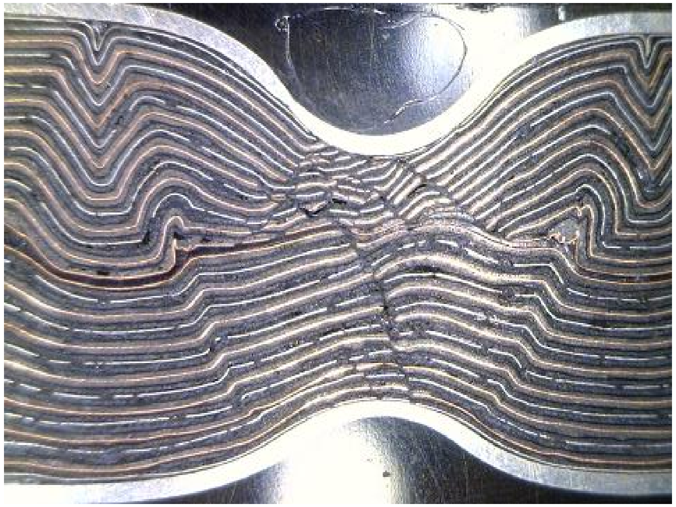
- The new release of software has reduced the simulation time by 50%.
- New test case of coupled simulation for hybrid pulse power characterization of the battery module.

Milestones (FY17)

IDs indicate whether milestones are primarily experimental (E), computational (C), or integrated (I).							
ID	FY17	Lead	Q1	Q2	Q3	Q4	Status
I.3	Demonstration of ability to construct 3D meshes of electrodes using reconstructions from micro-tomography	SNL	P				Complete
E.3	Potential-dependent solid diffusivities for Li-ion and EIS	LBNL		P			Complete
I.4	Demonstrated ability of VIBE/OAS to simulate onset of short-circuit due to mechanical abuse informed by microstructure	ORNL		D			Complete
E.4	Data from mechanical deformation tests	ORNL			P		Ongoing
C.2	Validated constitutive models and failure criteria for electrode materials and spirally wound, wound prismatic, and stacked electrodes under indentation	ORNL				P	Ongoing
I.5	Deployment of VIBE/OAS with integrated multiscale capability	ORNL				S	Ongoing

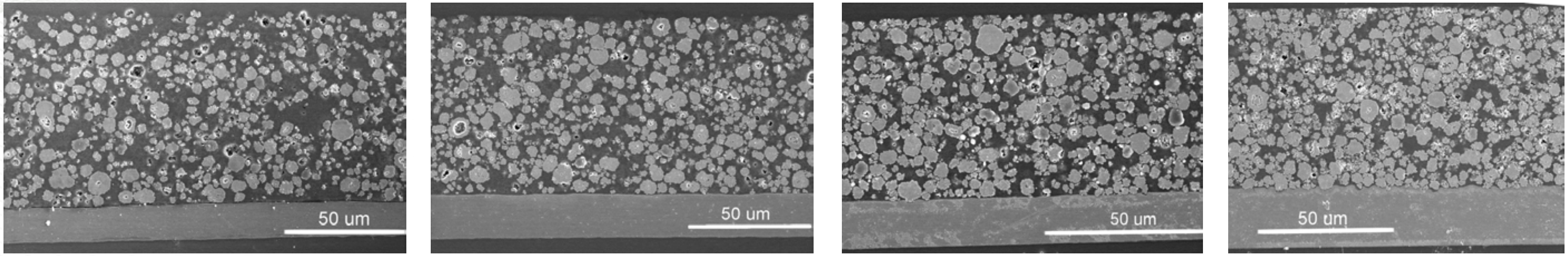
Approach: Microstructure changes during mechanical indentation

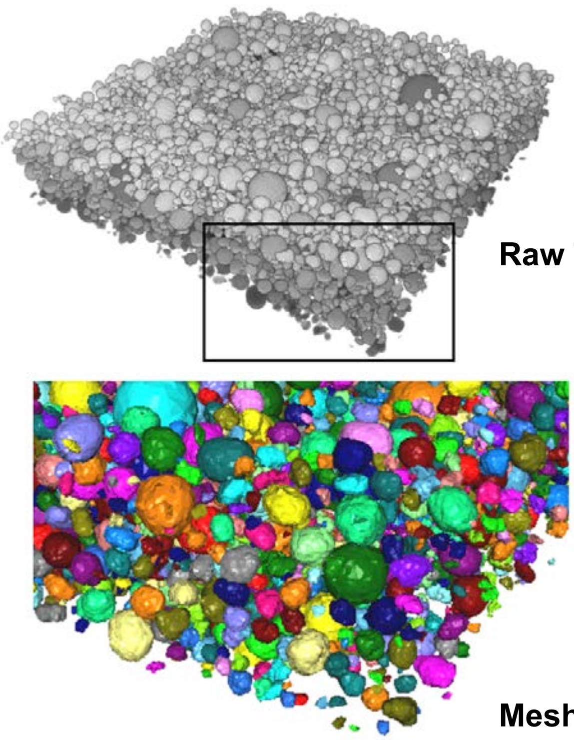




- Single side indentation or pinch test
- Understand electrode particle reorganization under compression
- Binder distribution and adhesion plays a significant role during failure
- Effects the transport properties that influences the cell behavior

Approach: Upscaling effective properties from microstructure simulation



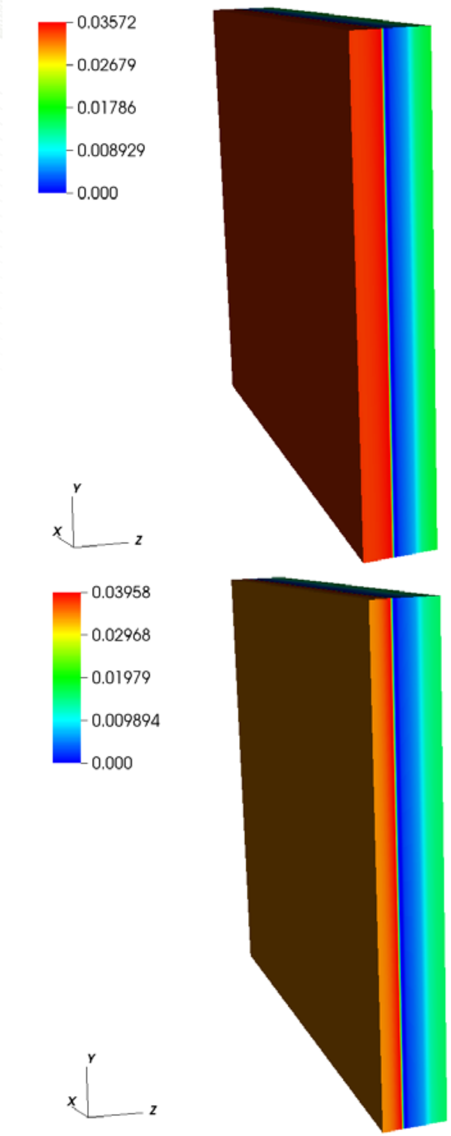


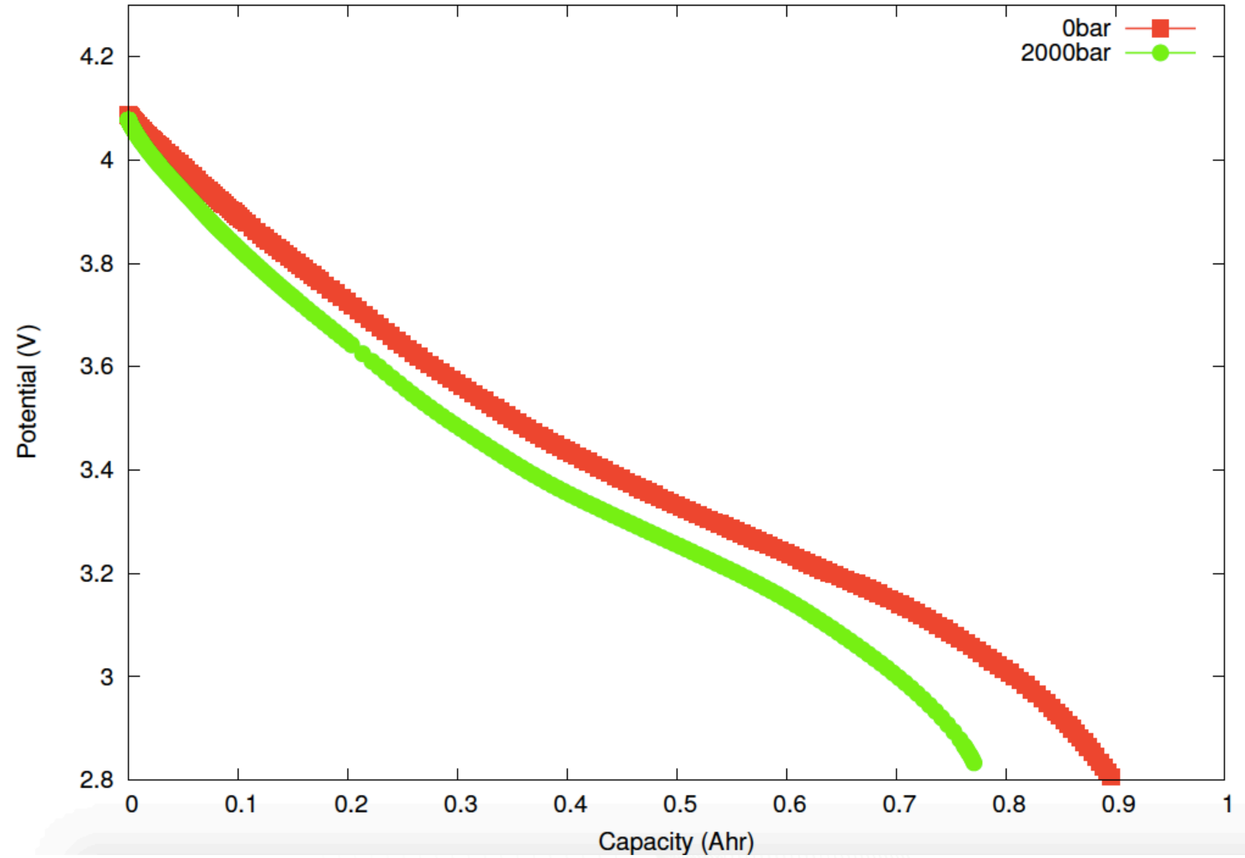
Raw Tomography

Meshed Particles

Pressure	Porosity	Mean (S/cm)
0 bar	0.478	0.001780646
300 bar	0.422	0.001982311
600 bar	0.436	0.001738324
2000 bar	0.26	0.002367756

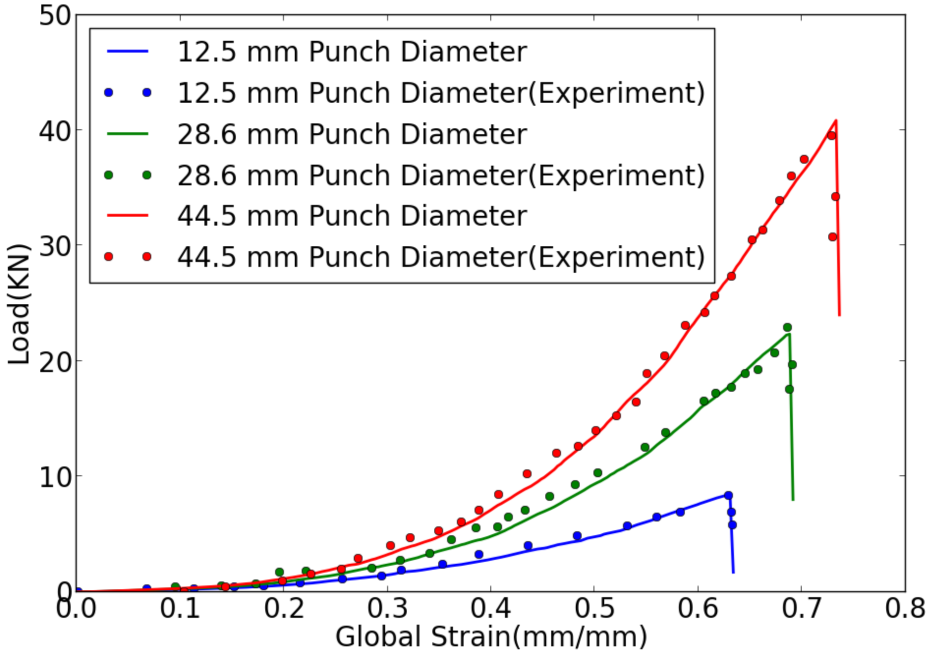
Technical Accomplishments: Electrodes calendared at various pressures

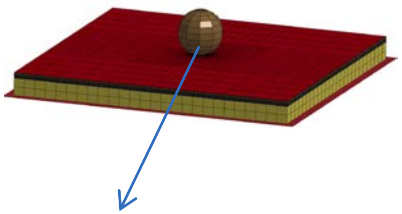




Capacity extracted under constant current discharge of NMC electrodes

Technical Accomplishments: Effect of Indenter Diameter-Modeling internal short

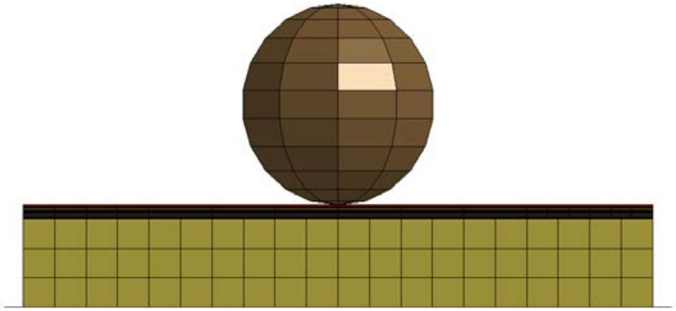




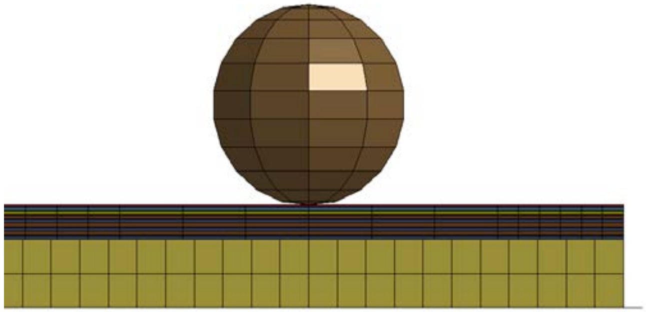
Indenter diameter varied from 12.5 mm to 44.5 mm

- Estimated failure criteria for separator using small indenter (12.5 mm diameter)
- Used the critical parameter to predict failure for 2 different size of indenter 28.6 and 44.45

Technical Accomplishments: Effect of Electrode thickness-Modeling internal short

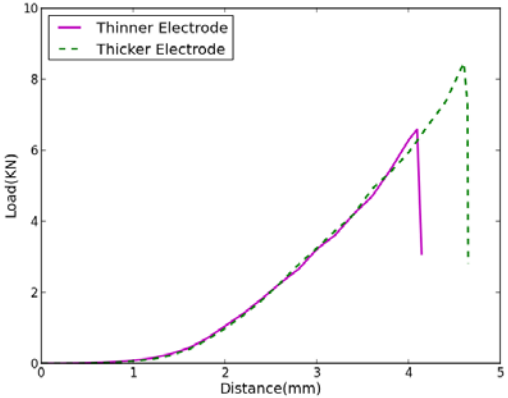


Thinner Electrode



Thicker Electrode

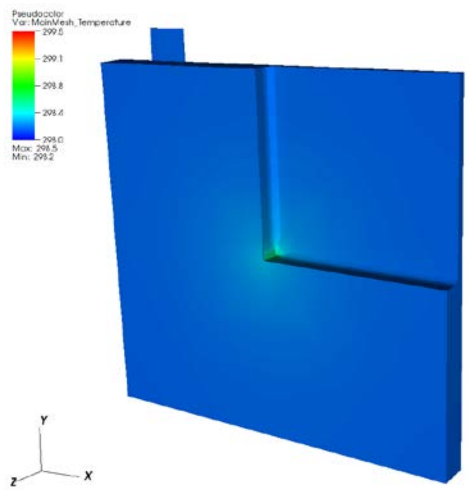
•In both the cases first 4 layers are resolved (Total number of layers with thin electrode ~ 28 and thick electrode ~ 12). Total height of the cell is 6.507 mm



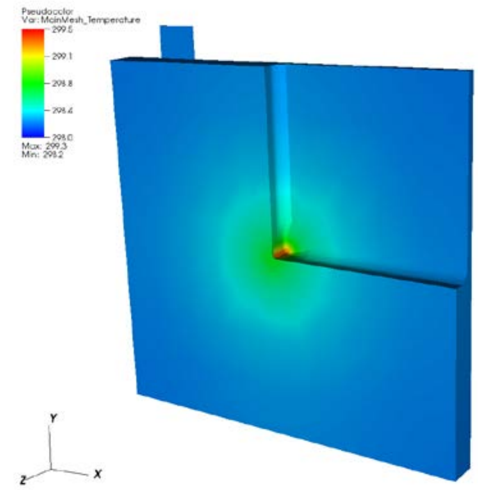
Case	Contact Area (mm^2)
Thinner-Electrode	0.53
Thicker Electrode	0.69

•Separator elements where the damage criterion (strain exceeds threshold of 50%) are tracked to obtain the total area of contact

Technical Accomplishments: Temperature distribution for different shorting areas



- 2x2 mm short area
- Potential drops instantaneously
- In-plane concentration gradients develop
- Temperature hot-spots are generated due to intercalation reaction local to area of short



- 4x4 mm short area
- Potential drops instantaneously
- In-plane concentration gradients develop
- Increase in area of short increases the heat generation

Summary Milestone-I.4 (Status: Complete)

Goals

- Conduct microstructure simulations
  - Upscaling effective transport properties
- Capability to simulate Onset of electrical short
  - Coupled Mechanical-electrochemical-thermal simulations
- Design experiments to generate validation data

Approach / Strategy

- Estimate appropriate binder location
- Upscale properties at varying pressures
- Simulate short from mechanical induced deformations

Results

- Separator failure criterion and effective contact area dictates the severity of short
- Microstructure reorganization under mechanical loading influences the effective transport properties.

Responses to Previous Year Reviewers' Comments

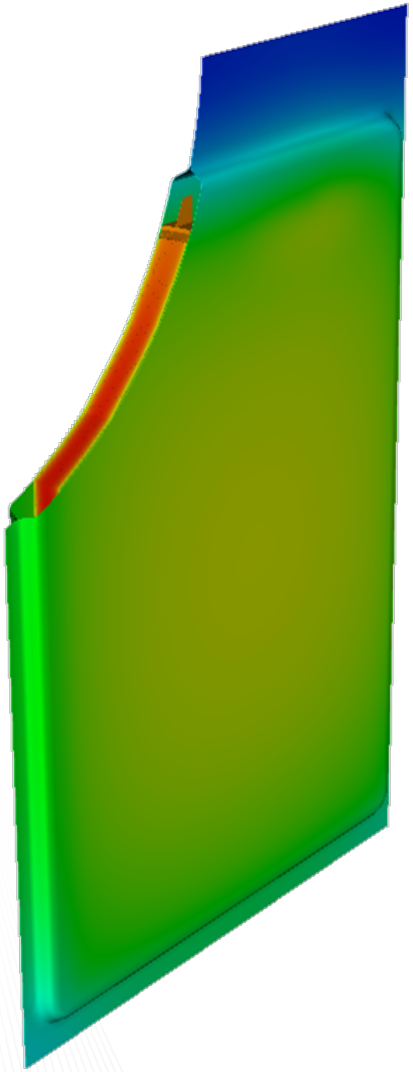
AMR 2016 Review Comments	Response
"to this reviewer, who also inquired whether there is any possibility for this project to leverage other, on-going CAEBAT III"	Monthly testing group meeting with NREL team. Exchanging experimental data for characterizing the battery modules.
"to this reviewer: whether it will be useful to academic researchers without access to these large commercial codes; the level of necessary detail to reproduce results in baseline performance modeling;"	Standard VIBE release consists of prebuild libraries of various open source physics based solvers that users can access through interface provided without the need for commercial license.
"This reviewer offered that one area of concern is the project team needs to have a more robust methodology to validate the completed models."	A comprehensive test matrix was developed and followed with current experiments planned at ORNL and NREL. These data sets will be used to validate the coupled simulations conducted.

Collaboration and Coordination with Other Institutions

- Collaboration with SNL (CABS sub) to bring microstructure modeling capabilities into VIBE/OAS
- Collaboration with LBNL/ANL (CABS sub) to refine tomography imaging data for simulations
- Monthly testing user group meeting with NREL to exchange experimental data for validation of dynamic discharge of battery module
- Collaboration with FORD (Prime) to develop multi-physics simulation tool to predict response under mechanical impact in LS-Dyna
- Active project with NHTSA on characterization experiments and simulations to develop crashworthiness models.

Remaining Challenges and Barriers

- Binder distribution and adhesion to the electrode particles
  - binder resolution with tomography imaging
  - bonding strength between binder/electrode particles
- Predicting the critical temperature threshold leading to thermal runaway
  - insufficient understanding of complete chemical mechanisms during runaway
- Electrochemical cycling of the NMC/Graphite electrodes under deformed configurations
  - uncontrolled experiments could lead to internal-short due to Li plating



Any proposed future work is subject to change based on funding levels

Proposed Future Research

- Reduced order modeling of dynamic discharge profiles.
- Understanding the influence of temperature variations during US06 dynamic discharge causing SOC non-uniformity in battery module
- Upscale effective properties under varying porosities and binder re-allocation
- Complete integration of microstructure models from SNL into VIBE/OAS
- Implement closure models from surface energy characterization to predict slip bands at the electrode scale

Any proposed future work is subject to change based on funding levels

Summary

Objectives

- Software design updates to improve VIBE computational performance
- Capability to simulate dynamic discharge
- Conduct micro-structure simulations to upscale effective transport properties
- Capability to simulate onset of electrical short using coupled mechanical-electrochemical-thermal simulations

Approach

- Launch component as daemon for continuous execution of physics based solver
- Python component wrapper translates calls from driver into messages to daemon
- Estimate appropriate binder location
- Upscale properties at varying pressures
- Simulate short from mechanical induced deformations

Accomplishments and progress

- New release of VIBE has reduced the simulation time by 50%.
- Algorithmic and software design improvements that allows for seamless integration and deployment via docker container
- Implemented variable potentio-static, galvano-static and open circuit voltage(OCV) resting conditions
- Separator failure criterion and effective contact area dictates the severity of internal short
- Microstructure reorganization under mechanical compression influences the effective transport properties during onset of short.

Future work

- Understanding the influence of temperature variations during dynamic discharge of battery module
- Implement closure models from surface energy characterization to predict slip bands at the electrode scale

Technical Back-Up Slides

Technical Accomplishments: Baseline simulation profiling

Time Step	NTG	TH:	EL:	TH:PO	TH: PI	NTG:PO	NTG:PI	EL:PO	EL:PI	Total
1	1.83	87.23	80.22	2.56	2.3	3.75	2.33	2.43	2.33	**184.98**
2	1.77	88	80.06	2.55	2.29	3.97	2.3	2.43	2.29	**185.66**
3	1.85	88.14	79.69	2.55	2.46	3.74	2.28	2.61	2.29	**185.61**
4	1.8	87.66	80.18	2.52	2.32	3.72	2.3	2.6	2.31	**185.41**
5	1.75	87.85	80.86	2.52	2.32	3.7	2.3	2.47	2.31	**186.08**
6	1.8	88.12	79.81	2.53	2.47	3.7	2.26	2.41	2.24	**185.34**
7	1.9	96.44	80.93	2.61	2.78	3.83	2.33	2.49	2.38	**195.69**
8	1.79	87.76	79.9	2.6	2.31	3.71	2.3	2.46	2.32	**185.15**
9	1.98	87.64	79.93	2.52	2.39	3.73	2.34	2.47	2.31	**185.21**
Total	**16.47**	**798.84**	**721.58**	**22.96**	**21.64**	**33.85**	**20.74**	**22.37**	**20.78**	**1679.23**
%	**0.95%**	**45.91%**	**41.47%**	**1.32%**	**1.24%**	**1.95%**	**1.19%**	**1.29%**	**1.19%**	**96.51%**

Driver Setup	Solve	Compute T Average	Total
56.678	12.156	13.403	82.237
56.904	12.184	13.54	82.628
57.213	12.17	13.33	82.713
56.622	12.189	13.45	82.261
56.813	12.187	13.4	82.4
56.772	12.179	13.67	82.621
57.005	12.18	18.84	88.025
56.735	12.178	13.36	82.273
56.565	12.194	13.43	82.189

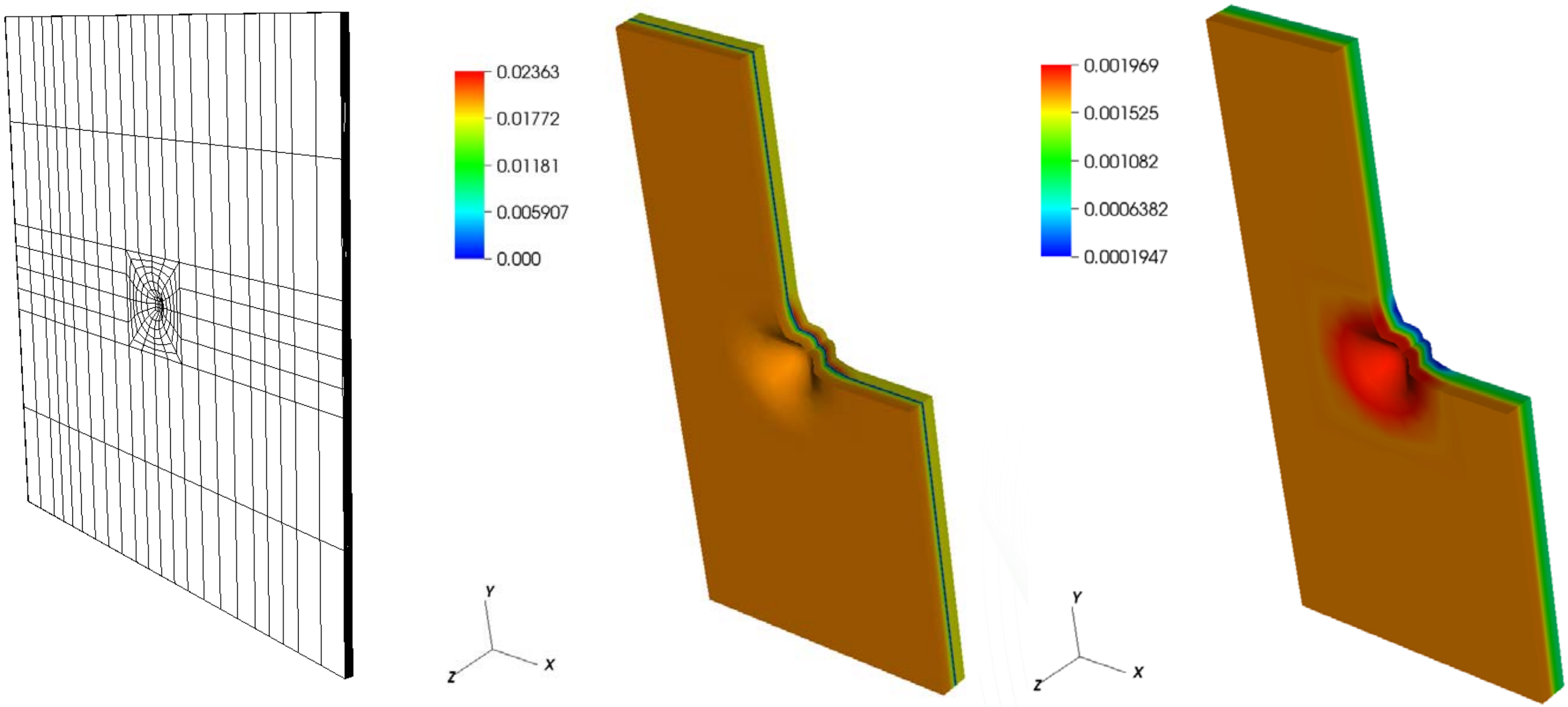
Driver Setup	Solve	Compute Sources	Total
38.29	8.7	28.9	75.89
38.26	8.688	28.8	75.748
37.557	8.702	29.078	75.337
38.253	8.691	28.873	75.817
38.118	8.702	28.783	75.603
37.9	8.688	28.815	75.403
37.849	8.704	29.963	76.516
37.839	8.689	28.938	75.466
38.104	8.689	28.819	75.612

Coupled simulations to understand the influence of property variations

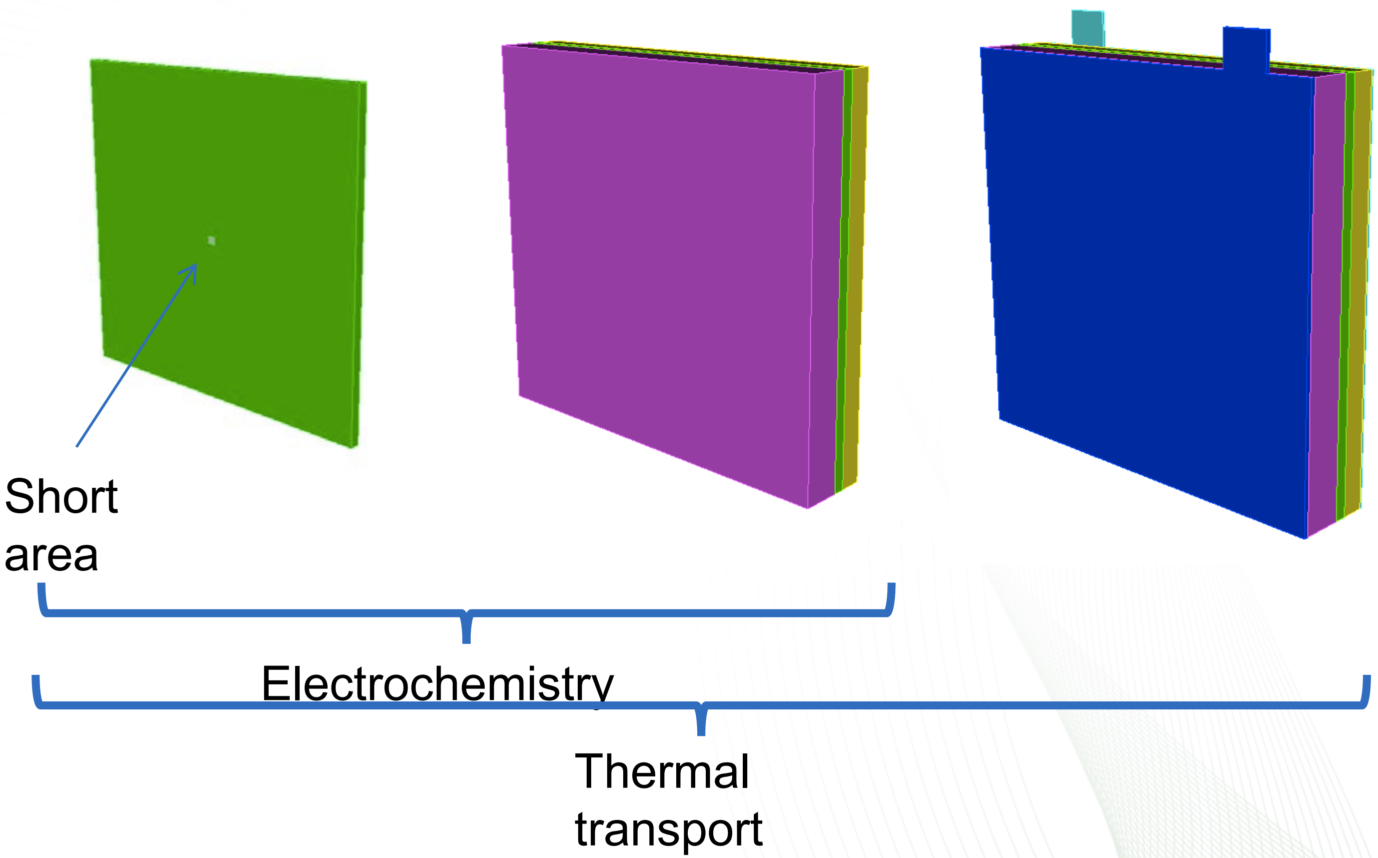
Symbol	Units	Anode (Carbon)	Separator	Cathode (NMC)
L	μm	133	25	100
ε_s	-	0.71	-	0.62
ε_e	-	0.26	0.48	0.29
ε_f	-	0.026	-	0.073
$c_s^{\max}$	mol/m^3	30813	-	51000
c_s^0	mol/m^3	20469	-	13872
c_e^0	mol/m^3		1300	
D_s	m^2/s	2.0x10^(-14)	-	7.5x10^(-10)
D_e	m^2/s		7.0x10^(-11)	
i_0	A/m^2	1.1	-	0.8
α_a	-	0.5	-	0.5
α_c	-	0.5	-	0.5
t_+^0	-		0.363	
σ	S/m	4.33	-	0.512
R_s	μm	6.35	-	5.15

1. Electrodes calendared at various pressures (same loading)
2. Deformed Electrodes (varying volume fractions of solid/liquid phase)

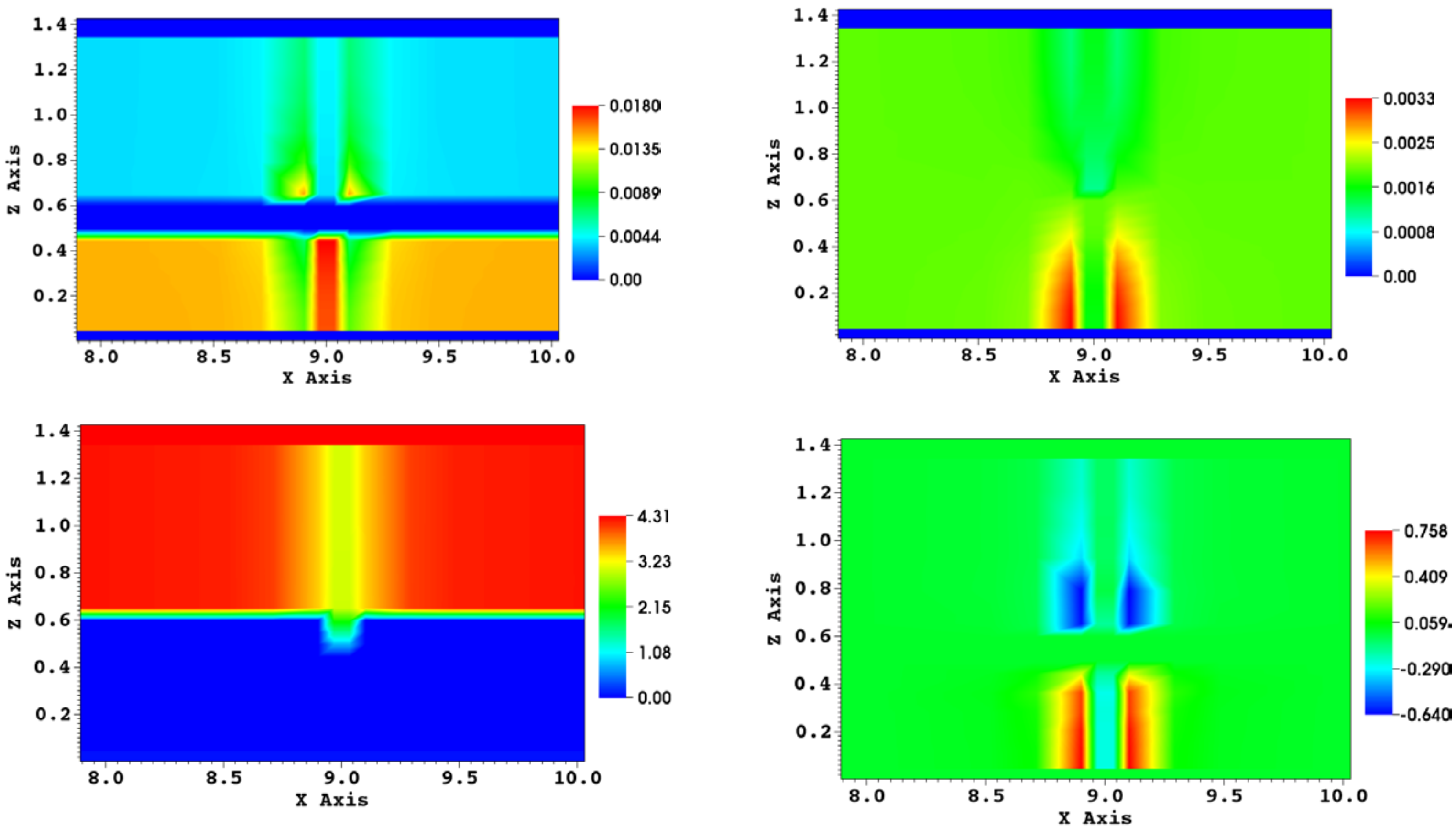
Deformed Electrodes (varying volume fractions of solid/liquid phase)



Technical Accomplishments: Construction of Cell (manually inducing the short)



Technical Accomplishments: Cross section across internal short at the end of 20sec



ECS Prime, 2016, Honolulu

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- Allu, S., Kalnaus S., Kumar A., Pannala S., Simunovic S., Wang H., and Turner J.A. "*A Computational Analysis of Battery Response during Onset of Internal Short Under Mechanical Abuse Conditions*." In *Meeting Abstracts*, no. 6, pp. 891-891. The Electrochemical Society, 2016.
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- Kumar, A., Kalnaus S., Simunovic S., Gorti S., Allu S., and Turner J.A. "*Communication—indentation of Li-ion pouch cell: Effect of material homogenization on prediction of internal short circuit.*" *Journal of The Electrochemical Society* 163, no. 10 (2016): A2494-A2496.
- H. Wang, A. Kumar, S. Simunovic, S. Allu, S. Kalnaus, J. A Turner, J. C Helmers, E. T Rules, C. S Winchester, P. Gorney, Progressive mechanical indentation of large-format Li-ion cells, *J. Power Sources*, 341 (2017) 156-164.